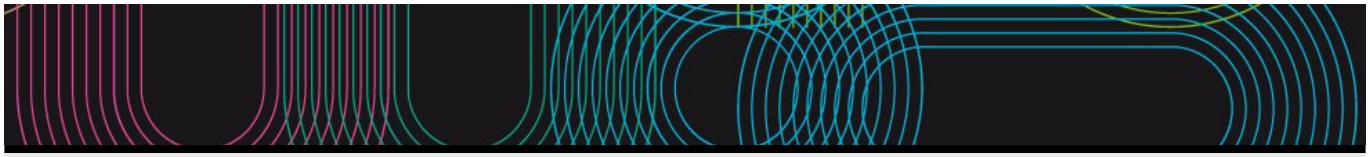

IDENTIFYING DATA

Physical chemistry I: Chemical thermodynamics

Subject	Physical chemistry I: Chemical thermodynamics			
Code	V11G201V01203			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	1st
Teaching language	Spanish Galician			
Department				
Coordinator	Fernández Nóvoa, Alejandro			
Lecturers	Fernández Nóvoa, Alejandro González Cabaleiro, Lara Otero Martínez, Clara Tojo Suárez, María Concepción			
E-mail	afnovoa@uvigo.es			
Web				
General description	The subject "Physical Chemistry I" is one of the first contacts of the students of the "Degree in Chemistry" with Physical Chemistry. This discipline studies the properties and behavior of chemical systems using the methods of Physics. The subject deals with the rigorous macroscopic treatment of chemical systems in equilibrium, systems already introduced in the subject "Chemistry II". Taking advantage of the basic knowledge of the principles of Thermodynamics, they will be applied to systems of chemical interest to have a quantitative description of them. For this quantitative treatment it is essential to be familiar with the differential calculus of more than one variable and the integral calculus of one variable, aspects addressed in the subject "Mathematics I". The knowledge about the macroscopic description of the chemical systems that will be achieved in this subject is complemented with the contents of the "Physical Chemistry II" of the second semester and with the subject "Physical Chemistry V" of the third year.			

Training and Learning Results

Code	
A1	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
B1	Ability for auronomous learning
B3	Ability to manage information
C11	Know the principles of Thermodynamics and its applications in Chemistry
C13	Know the principles and applications of electrochemistry
C28	Interpret data derived from laboratory observations and measurements in terms of their meaning and relate them to the appropriate theory
C29	Demonstrate ability for numerical calculations and interpretation of experimental data, with correct use of units and estimation of uncertainty
D1	Ability to solve problems
D3	Ability to communicate in both oral and written form in Spanish and / or Galician and / or English

Expected results from this subject

Expected results from this subject	Training and Learning Results			
Explain the energetic exchanges in the thermodynamic systems in function of the changes in the variables of state.	A1	B1 B3	C11 C28 C29	D1 D3

Establish if a thermodynamic process that is spontaneous or not from the calculation of the variations of the thermodynamic properties.	A1	B1 B3	C11 C29	D1 D3
Handle thermodynamic tables to obtain values of the functions of thermodynamic state of reaction to different temperatures.	A1	B1 B3	C11 C28 C29	D1 D3
Determine the thermodynamic characteristics of a change of phase, and know the interval of applicability of the equations employed	A1	B1 B3	C11 C29	D1 D3
Calculate the thermodynamic properties of an ideal solution from his composition	A1	B1 B3	C11 C29	D1 D3
Analyse the colligative properties of a solution from the concentration of the solute and the properties of the dissolvent.	A1	B1 B3	C11 C28 C29	D1 D3
Describe of the behaviour of the real solutions employing the concepts of activity and coefficient of activity and be able to calculate them from experimental data and theoretical models.	A1	B1 B3	C11 C28 C29	D1 D3
Calculate the thermodynamic constant of reactions, from the concentrations or activities of the species and relate it with the thermodynamic functions.	A1	B1 B3	C11 C13 C28 C29	D1 D3

Contents

Topic	
The laws of the Thermodynamic in Chemistry.	First Law of Thermodynamics. Internal energy. Enthalpy. Heat capacities . Thermochemistry. Second law of Thermodynamics. Entropy. Third law of Thermodynamics.
Thermodynamic functions.	Gibbs Equations. Maxwell relationships. Calculation of variations of the state functions . Partial Molar quantities. Chemical potential of ideal and real gases.
Phase equilibrrium in one component systems.	Phases Rule. First order transitions. Clapeyron and Clausius-Clapeyron Equations.
Ideal Solutions.	Molar partial Volume. Ideal solutions: Raoult's law. Ideal diluted solutions: Henry's Law. Colligative Properties
Non-ideal Solutions.	Deviations of the Raoult's law. Activity and activity coefficient . Electrolitic solutions. Debye-Hückel theory.
Chemical equilibrium.	Equilibrium in gas phase reactions. Response of equilibrium to temperature and pressure changes. Acid-base equilibria. Solubility Product. Electrochemical systems.
Laboratory Practices.	- Experimental determination of equilibrium constants using spectrophotometric or potentiometric techniques. - Experimental determination of enthalpies of combustion, dissolution, neutralization, fusion or vaporization. - Experimental determination of colligative properties.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	24	33	57
Seminars	24	33	57
Laboratory practical	14	2.5	16.5
Problem and/or exercise solving	0	8.5	8.5
Self-assessment	0	4	4
Essay questions exam	2	0	2
Essay questions exam	0	0	0
Report of practices, practicum and external practices	0	5	5

*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies

	Description
Lecturing	They will consist of an exposition by the teacher of the fundamental aspects of each topic, based on the material available on the MOOVI platform. Numerical problems will also be formulated to help understand and settle concepts.
Seminars	The seminar classes will be devoted mainly to solving problems and, when necessary, to delve into the aspects of the topics that present the greatest difficulties for the students.

Laboratory practical	Carrying out, under the supervision of the teaching staff but independently, of laboratory practices in sessions of 3.5 hours. With enough time in advance, the students will have the scripts for the practices to be carried out on the MOOVI platform, along with all the additional material necessary. The script will present the essential elements to carry out the practice at an experimental level, as well as the basic points of its theoretical foundation and data treatment. At the end of the practices, and within the term set by the teaching staff, it will be necessary to deliver the report of one of them, prepared following the guidelines given by the teaching staff.

Personalized assistance

Methodologies	Description
Lecturing	In the teacher's tutoring schedule, those doubts of the students that may arise throughout the course in the theory classes will be resolved individually and more personally.
Seminars	In the teacher's tutoring schedule, those doubts of the students that may arise throughout the course in the seminar classes will be resolved individually and more personally.
Laboratory practical	In the teacher's tutoring schedule, those doubts of the students that may arise during the course in the laboratory classes or during the preparation of the corresponding practical reports will be resolved individually and on a more personal basis.
Tests	**Description**
Essay questions exam	In the teacher's tutoring schedule, those doubts of the students that may arise throughout the course during the preparation of the first written exam will be resolved individually and more personally.
Report of practices, practicum and external practices	In the teacher's tutoring schedule, those doubts of the students that may arise during the course in the laboratory classes or during the preparation of the corresponding practical reports will be resolved individually and on a more personal basis.
Essay questions exam	In the teacher's tutoring schedule, those doubts of the students that may arise throughout the course during the preparation of the second written exam will be resolved individually and more personally.

Assessment

	Description	Qualification	Training and Learning Results
Laboratory practical	It marks here together with the effort and the attitude, the skills and the competitions developed by the students during the realisation of the distinct practical. Attendance at the practical sessions is mandatory and, therefore, it is not possible to pass the subject if it is not completed.	10	A1 B1 C11 D1 B3 C28 D3 C29
Problem and/or exercise solving	In addition to the problem bulletins, at the end of each topic or group of topics, some "Assessable Exercises" will be proposed. The students must solve them independently and deliver within the deadline set by the teaching staff.	12.5	A1 B1 C11 D1 B3 C13 D3 C29
Self-assessment	At the end of each topic, students will have the possibility of answering, through the MOOVI platform, a self-correcting "Self-Assessment Test".	7.5	A1 B1 C11 D1 B3 C13 D3 C29
Essay questions exam	There will be a written exam halfway through the semester on the date approved by the Faculty Board. This test will cover the contents of subjects I, II and III.	32.5	A1 B1 C11 D1 B3 C29 D3
Essay questions exam	A written exam will be carried out at the end of the semester on the date approved by the Faculty Board (the date will coincide with that of the Global Test for students of the Global Assessment modality). This test will cover the contents of subjects IV, V and VI.	32.5	A1 B1 C11 D1 B3 C13 D3 C29
Report of practices, practicum and external practices	The report of a practice proposed by the teaching staff will be made, which must be presented taking care of the formal aspects related to the organization, the correct use of the units, the correct preparation of the graphics and the presentation of the results. The critical analysis of these and drawing conclusions will also be valued.	5	A1 B1 C11 D1 B3 C28 D3 C29

Other comments on the Evaluation

Continuous assessment:

- The voluntary work of the student ("*Self-assessment Test*" and "*Evaluable Exercises*") may constitute up to 20% of the final grade provided that the student performs at least half of the activities proposed throughout the course. course.
- To pass the subject, it is an essential requirement that the average of the marks in the written exams be equal to or

greater than 4.0 out of 10.0 points. In the case of not reaching said score, the qualification that will be reflected in the minutes will only be the average of the qualifications of the tests, not counting any of the other sections.

- To pass the subject, it is an essential requirement to carry out the laboratory practices and obtain in them a minimum global qualification of 5.0 out of 10 points (66.7% laboratory work, 33.3% report). In the case of not reaching said score, the grade that will be reflected in the minutes may not exceed 4.0 points.
- Attendance to the practical sessions is mandatory and, therefore, it is not possible to pass the subject if it has not been done.
- To pass the subject, it is an essential requirement to obtain a grade equal to or greater than 5.0 points out of 10 in its overall grade (10% laboratory practices, 12.5% evaluable exercises, 7.5% self-assessment questionnaires, 65% written tests and 5% practice reports).

Overall evaluation:
Students who, within the term set by the Faculty, opt for the Global Assessment modality, will take a global written exam on the date set by the Xunta de Facultade. This overall written test will account for 85% of the grade for the subject.
In this global evaluation, the Laboratory Practices will constitute 10% of the qualification of the subject and 5% the corresponding reports.
- To pass the subject, it is an essential requirement to obtain a grade equal to or greater than 4.0 out of 10.0 in the overall written exam. In case of not reaching said score, the qualification that will be reflected in the minutes will only be the qualification of the global test, not counting any of the other sections.
-To pass the subject, it is an essential requirement to carry out the laboratory practices and obtain an overall minimum grade of 5.0 out of 10 points (66.7% laboratory work, 33.3% report). In the case of not reaching said score, the grade that will be reflected in the minutes may not exceed 4.0 points
- To pass the subject, it is an essential requirement to obtain a grade equal to or greater than 5.0 points out of 10 in its overall grade (85% overall test, 10% laboratory practices and 5% practice reports).
Examined/Not Examined Status:The participation of the students in one of the two written tests or the attendance of more than two laboratory sessions will imply the condition of "taked exam" and, therefore, the assignment of a qualification.
Second opportunity:In the case of the Continuous Evaluation for the evaluation of the second opportunity, the qualifications of the "*Evaluable Exercises*", of the "*Self-assessment Test*", of the laboratory practices and of the corresponding reports will be maintained.

In the case of the Global Evaluation for the evaluation of the second opportunity, the qualifications of the laboratory practices and the corresponding reports will be maintained.

Sources of information

Basic Bibliography

Levine, I. N., **"Principios de Fisicoquímica"**, 6ª Ed, McGraw-Hill Education, 2014
Engel, T.; Reid, P., **"Química Física"**, 1ª Ed, Pearson, Adison Wesley, 2006
Atkins, P.W.; De Paula, J., **"Química Física"**, 8ª Ed, Editorial Médica Panamericana, 2008

Complementary Bibliography

Levine, I.N., **"Problemas de Fisicoquímica"**, 1ª Ed, McGraw-Hill Interamericana, 2005
Rodríguez Renuncio, J.A., **"Termodinámica Química"**, 2ª Ed, Síntesis, 2000
Rodríguez Renuncio, J.A., **"Problemas resueltos de Termodinámica Química"**, 1ª Ed, Síntesis, 2000
Chang, R., **"Fisicoquimica"**, 3ª Ed, McGraw-Hill Interamericana, 2008
Metz, C.R., **"Fisicoquímica. Problemas y Soluciones"**, 1ª Ed, McGraw-Hill Interamericana, 1991

Recommendations

Subjects that continue the syllabus

Physical Chemistry II: Surfaces and Colloids/V11G201V01208
Physical Chemistry V: Chemical Kinetics/V11G201V01308

Subjects that it is recommended to have taken before

Mathematics: Mathematics 1/V11G201V01103
Chemistry: Chemistry 2/V11G201V01109